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H. Lee Nguyen
Lewis Research Center
Cleveland, Ohio

and

Ming-Jyh Wey
MBR Combustion Research Incorporated
Princeton, New Jersey

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EVALUATION OF A HYBRID KINETICS/MIXING-CONTROLLED COMBUSTION MODEL
FOR TURBULENT PREMIXED AND DIFFUSION COMBUSTION USING KIVA-II

H. Lee Nguyen*
National Aeronautics and Space Administration
Lewis Research Center
Cleveland, Ohio 44135

and

Ming-Jyh Wey
MBR Combustion Research Incorporated
Princeton, New Jersey 08540

SUMMARY

Two-dimensional calculations were made of spark-ignited premixed-charge combustion and direct-injection stratified-charge combustion in gasoline fueled piston engines. Results are obtained using kinetic-controlled combustion submodel governed by a four-step global chemical reaction or a hybrid laminar kinetics/mixing-controlled combustion submodel that accounts for laminar kinetics and turbulent mixing effects. In this work, the numerical solutions are obtained by using KIVA-II computer code. The KIVA-II code uses a kinetic-controlled combustion submodel governed by a four-step global chemical reaction; (i.e., it assumes that the mixing time is smaller than the chemistry). Our efforts involved the implementation of a hybrid laminar/mixing-controlled combustion submodel of Abraham et al. into KIVA-II. In this model, chemical species approach their thermodynamics equilibrium with a rate that is a combination of the turbulent-mixing time and the chemical-kinetics time. The combination is formed in such a way that the longer of the two times has more influence on the conversion rate and the energy release. An additional element of the model is that the laminar-flame kinetics strongly influence the early flame development following ignition.

Future efforts involve the implementation of this hybrid combustion model to study the combustion processes in High Speed Civil Transport engines and small gas turbine engines and to better predict NO_x emission and unburned hydrocarbon.

INTRODUCTION

The overall objective of this research is to implement a state-of-the-art laminar and turbulent combustion model into a three-dimensional compressible Navier-Stokes code. The KIVA-II code has been chosen for use in the present work since it is the most developed of the available multi-dimensional combustion computer programs for application of the in-cylinder combustion dynamics of internal combustion engines. There are features of KIVA-II that make it well suited for other applications as well, for example gas turbine combustors. By starting from an existing code KIVA-II and implementing an existing hybrid laminar kinetics/mixing-controlled combustion model of Abraham et al. (ref. 1)

*Member AIAA.

into KIVA-II and assessing the accuracy of this hybrid combustion model by comparisons between predictions obtained from kinetic-controlled and hybrid laminar/mixing-controlled combustion models, results can be obtained at much earlier dates. Furthermore, this hybrid combustion model has already been applied successfully to predict spark-ignited spray combustion in a rotary engine (refs. 1 to 3) and premixed-charge combustion in reciprocating engines (ref. 4). In this work, predictions are obtained for both spark-ignited premixed-charge and Direct-Injection Stratified-Charge combustion in gasoline fueled piston engines. The results of this study will be utilized in future works which will involve the implementation of this hybrid combustion model and its extension to include multi-step chemical reactions and chemical species to study the combustion processes in gas turbine combustors. This is part of an effort to develop/use advanced computer models to analyze and design combustor components and subcomponents, understand the physics and determine how to optimize the design to improve the performance of High Speed Civil Transport engine and small gas turbine engine combustors.

Recent advances in high-speed and large-memory computers, numerical algorithms, grid generation, and mathematical modelling of turbulent reactive flows have markedly expanded the horizon of turbulent reactive flows that can be studied by numerical methods. However, full numerical simulation (or direct simulation of turbulence) and large-eddy simulation of a simple turbulent flame model still require a great deal of computer time and memory. Thus, it is necessary to introduce models into the codes for processes that occur on time and length scales that are too short to be resolved on the grid and time step used by the code. The use of models to describe unresolved physical processes introduces some empiricism into the calculations and the validity of the models can be assessed by comparison with experimental data.

Combustion processes and modelling has typically been treated by means of (1) complete reaction-rate models, (2) eddy-breakup and mixing-controlled models, (3) equilibrium chemistry, and (4) finite-rate chemistry (or kinetic-controlled) models. In complete reaction models (ref. 5), it is assumed that instantaneous reaction occurs at any region where both fuel and air are present; the extent of the reaction is determined by the stoichiometric limit, i.e., the amount of fuel present determines the extent of the reaction under fuel-lean conditions, whereas the amount of oxygen determines the extent of the reaction under fuel-rich conditions. Complete reaction models are mixing-controlled and assume that the mixing time is much longer than the characteristic chemical kinetics time. This assumption may not be valid in the recirculation zones, and near solid walls such as combustor walls. However, if the flow is decelerated and the pressure and temperature increase so that reactions can proceed faster than mixing processes, a flame may be formed which is controlled by mixing and diffusion.

Equilibrium chemistry models (ref. 6) reduce the number of conservation equations for the chemical species to be solved. It is assumed that the chemical kinetics time is zero and reactions are mixing-controlled so that as soon as fuel and oxidizer are present at the same region, reactions occur as long as the mixture is within its flammability limits.

In eddy-breakup models, the reaction rate is determined by the entrainment of fuel and oxidizer into the flame front. This entrainment depends on the local levels of turbulence, and the mean concentrations of fuel, oxidizer and

products, or the root-mean-square of the concentration fluctuations (refs. 7 and 8). One of the main drawbacks of eddy-breakup models is their inability to predict local chemical equilibrium. Local chemical equilibrium can be achieved by expressing the reaction rate as the ratio between a concentration difference and the mixing (or chemical) time (ref. 9). The concentration difference is to be interpreted as the difference between the local concentration and that corresponding to local chemical equilibrium at the same local temperature.

Finite-rate chemistry models assume that reaction rate is kinetics-controlled. These models assume that the mixing time is much smaller than the chemical kinetics time. These combustion models are not adequate when turbulent mixing is slower than the chemistry; however, they can be used satisfactorily to predict chemically controlled reactions (i.e., low temperature reactions, quenching, etc.). These models can be classified in two groups: global or quasiglobal and detailed chemistry models (refs. 10 and 11). Global models reduce the number of kinetic equations to be solved. However, these models may be able to predict qualitatively the average value of heat release and unable to predict local chemical equilibrium unless the reaction rates are expanded in Taylor series expansion around their local equilibrium values. Detailed chemical kinetics mechanisms are accurately known only for simple hydrocarbons, e.g., methane (ref. 12), propane (refs. 10, 11, and 13), and for hydrogen-oxygen combustion (ref. 14). For simple hydrocarbons, these mechanisms involve about several hundred chemical reactions and numerous chemical species, and have only been used to predict simple flows (e.g., complete stirred reactors) (ref. 13), and one-dimensional flame propagation phenomena. These studies (e.g., well-stirred reactors computations) do not account for turbulence-chemistry effects and do not provide the flow field information. Nguyen and Ying used detailed propane chemical kinetics mechanisms to perform benchmark and sensitivity studies of spray combustion of two-dimensional gas turbine combustion (ref. 11).

Depending on the nature of the time scales involved in the chemical reactions occurring in different regions inside a combustor, the relative roles of chemical kinetics and mixing in turbulent combustion can be interpreted by the above combustion models for limiting cases of very fast or very slow reactions, where the chemical source terms and their relation to turbulent mixing can be modelled. In the present study, a hybrid laminar kinetics/turbulent mixing model of Abraham et al. (ref. 1) is implemented into KIVA-II, and this combustion model is tested on both premixed-charge combustion and direct-injection stratified-charge combustion in gasoline fueled piston engines. This hybrid combustion model selects the reaction rate within the combustion flow field region based on a comparison between the local chemical kinetics and mixing times. In gas turbine combustors and internal combustion engines, combustion would occur in both the kinetic- and mixing-controlled regimes in different combustor regions; therefore hybrid combustion models would be required to accurately predict the combustion flow field. In the current study, results obtained using hybrid combustion model are compared with predictions obtained using kinetic-controlled combustion model. In this work, the hybrid kinetics/mixing combustion model is limited to quasiglobal reaction mechanisms. However, detailed chemistry models would be included in future works.

PROBLEM FORMULATION

Engine descriptions. - The specifications and test conditions for the piston-cylinder configuration are listed in table I. For these calculations, the numerical grid consists of 20 grid points in the axial direction and 22 grid points in the radial direction. Both the direct-injection stratified charge and premixed-charge engine were tested at an overall equivalence ratio of about 1.0.

The calculations were made using the KIVA-II computer program, which solves three-dimensional equations of transient turbulent chemically reactive fluid dynamics with spray using an Implicit-Continuous Eulerian (ICE) technique for flow solver. The equations and the numerical method of solution are discussed in detail by Amsden et al. (ref. 15). Turbulence is modelled using the two-equation $k-\epsilon$ model equations. The standard turbulence model constants C_1 , C_2 , and C_3 (ref. 15) were used and their values are given in table II. A Bessel function velocity profile (ref. 15) was used to simulate the swirl velocity profile of the incoming air. Standard boundary conditions were used in this two-dimensional axisymmetric engine model and the details are described in reference 15. For the direct-injection stratified-charge gasoline engine cases, liquid fuel (isooctane) was injected starting at crankshaft angle 5.2° BTDC for an injection duration of 12.6° .

Details of the hybrid kinetics/mixing combustion model and modification of KIVA-II to implement this combustion model are reviewed in the following section.

Combustion models. - The hybrid kinetics-mixing controlled combustion model of Abraham et al. (ref. 1) was incorporated into KIVA-II. This combustion model simulates the growth of the initial flame kernel into a fully developed turbulent flame and its subsequent propagation. The reaction rates are proportional to the difference between the local concentrations and their corresponding equilibrium values and inversely proportional to a characteristic time required for the achievement of equilibrium. With this hybrid kinetics-mixing combustion model, the reaction rates are controlled by chemical kinetics (or turbulent mixing) if the characteristic mixing (or chemical kinetics) time is much shorter than the chemical kinetics (or mixing) time.

In the species conservation equation the time rate of change of species mass fraction due to conversion from one species to another is given by

$$\frac{dY_i}{dt} = - \frac{(Y_i - Y_i^*)}{\tau_c} \quad (1)$$

where Y_i is the mass fraction of species i and Y_i^* is the local and instantaneous thermodynamic equilibrium value of the corresponding mass fraction. The present hybrid kinetics-mixing combustion model considered isooctane oxidation including the formation of carbon monoxide and carbon dioxide. Seven chemical species were considered in the hybrid combustion model: C_8H_{18} , O_2 , N_2 , H_2O , CO_2 , CO , and H_2 . Nitric oxide was also accounted for in the present calculations. NO_x was assumed to be present only in trace amounts and was treated separately from the energy-releasing species. The NO_x model used was based on the extended Zeldovich mechanism (ref. 16). This model assumes that

the NO formation rate depends on the temperature, the local equilibrium composition of the C-O-H system, and the local NO concentration. Fuel-bound nitrogen NO_x is not considered in this model. Future works will attempt to extend the hybrid combustion model to incorporate more detailed reaction mechanisms including NO_x reactions and additional chemical species.

The characteristic time τ_c appearing in equation (1) for the achievement of equilibrium is assumed to be the sum of the local laminar kinetics time and the local turbulent mixing time. This ensures that the rates of conversion of reactants to products of the reactions considered are controlled by the longer of the local turbulent mixing or local laminar kinetics time

$$\tau_c = \tau_l + f\tau_t \quad (2)$$

The expressions for τ_l and τ_t are

$$\tau_l = B' \left(\frac{T}{T_0} \right)^\xi \left(\frac{P}{P_0} \right)^\eta \exp \left[\frac{Ea}{RT} (1 + C|\phi - 1.15|) \right] \quad (3)$$

and

$$\tau_t = C_{m_2} \frac{k}{\varepsilon} \quad (4)$$

if

$$\frac{C_{m_2}}{C_{m_3}} \frac{(Y_P - Y_{PS})}{(1 + S)(Y_F - Y_F^*)} \geq 1 \quad (5)$$

$$\tau_t = C_{m_3} \frac{k}{\varepsilon} [1 + S] \frac{Y_F - Y_F^*}{Y_P - Y_{PS}} \quad (6)$$

if

$$\frac{C_{m_2}}{C_{m_3}} \frac{(Y_P - Y_{PS})}{(1 + S)(Y_F - Y_F^*)} < 1 \quad (7)$$

where

$$S = \frac{(Y_{O_2} - Y_{O_2}^*)}{(Y_F - Y_F^*)}$$

The delay coefficient in equation (2) is equal to unity except during ignition, as will be discussed below. The constants of the laminar kinetics time equation (3), the function $(1 + C|\phi - 1.15|)$ and the constants B' , C , ξ , and η were obtained by calibrating computed and measured laminar flame speed over a range of equivalence ratios (ϕ), pressures (P), and temperatures (T). The kinetic constants used in this work are for isooctane (ref. 4) and they are given in Table II. T_0 and P_0 are reference temperature (298 K) and pressure (1 atm), respectively, ϕ denotes equivalence ratio. One laminar kinetics time was used for all the seven chemical species considered.

The turbulent mixing time in equations (4) and (6) is the same as that of Mangnussen and Hjertager (ref. 17), modified for the formulation of equation (1). The constants C_{m_2} and C_{m_3} are given in table II. The subscript

P denotes a sum over all of the products (CO , CO_2 , H_2 , and H_2O), and the subscript PS denotes the product sum at the time of the spark (ref. 4). Equations (4) and (6) used to describe the turbulent mixing time are generally applicable to diffusion as well as to premixed flames, and the local turbulent mixing time is controlled by the smaller of the fuel, oxygen, or products local concentrations. The subscripts F and O_2 denote fuel and oxygen, respectively. The superscript $*$ denotes local thermodynamic equilibrium value.

The delay coefficient f appearing in equation (2) has been given the following form

$$f = 1 - \exp \frac{(-t - t_s)}{\tau_d} \quad (8)$$

and

$$\tau_d = \frac{C_{m_1} \ell}{S_L} \quad (9)$$

$(t - t_s)$ is the time after spark, and the delay coefficient f sets the initial value of the conversion time τ_c equal to τ_0 (laminar kinetics time) and delay complete consideration of turbulent mixing until the time required for the laminar flame to traverse a distance equal to C_{m_1} times the length scale ℓ of the turbulent eddies (3),

$$\ell = C_\mu^{3/4} \frac{k^{3/2}}{\epsilon} \quad (10)$$

where $C_\mu = 0.09$ (3). The laminar flame speed S_L was given as (18)

$$S_L = B_m - B_2(\phi - \phi_m)^2 T_0^\alpha P_0^\beta (1 - 2.1 r) \quad (11)$$

where $\alpha = 2.18 - 0.8(\phi - 1)$, $\beta = -0.16 + 0.22(\phi - 1)$, r is the residual mass fraction, and the constants B_m , ϕ_m , and B_2 are 0.263, 1.13, and 0.847 for

isooctane (ref. 4). The delay time τ_d appearing in equation (8) accounts for spark ignition effect on laminar flame (ref. 19).

For this work, results obtained using chemical kinetics-controlled combustion model are calculated using the four kinetics reaction mechanisms (including the extended NO_x Zeldovich mechanism and six equilibrium reactions. These reactions and species are described in reference 20. Also, a fast algebraic solver, CHMQGM (ref. 15), was used to evaluate the local equilibrium species concentrations for the same equilibrium reactions (ref. 20) used in both calculations employed either hybrid combustion model or kinetics-controlled combustion model.

RESULTS AND DISCUSSION

Comparisons of combustion rate in a direct-injection stratified-charge gasoline fueled piston engine computed using kinetics-controlled combustion model (case 1) and hybrid combustion model (case 2) were made at various crankshaft angles (TDC is at 0). The comparisons were also made for a case involving hybrid combustion modelling of a premixed charge gasoline engine with same engine dimension (case 3). In all the cases studied, the simulations were started at the beginning of compression stroke and ended at the crankshaft angle of 65° ATDC.

Figure 1 shows the computed mean gas velocity, turbulent kinetic energy, and fuel spray at crankshaft angle about 29° BTDC for cases 1 to 3. The velocity vectors are similar for all three cases and are predominantly in the direction of the piston motion. Figure 1(b) shows the turbulent kinetic energy in the cylinder at the same crankshaft angle. Under each contour plot are the high (H) and low (L) values of the contours and the intervals of the lines that are between the H- and the L-lines. It may be seen that the turbulent kinetic energy is high for all the engine cases studied with the piston cup with a bowl. The added azimuthal swirl profile also enhances the turbulent kinetic energy. This would increase the vaporization, fuel-air mixing and burning rates. Figures 1(a) and (c) indicate that the regions of high turbulence levels increase the fuel vaporization rate. At crankshaft angle about 11° BTDC, 4° BTDC, and about TDC, the increase in density increases the turbulent kinetic energy as TDC is approached (see figs. 2(b), 3(b), and 4(b)). This would increase the burning rate and flame propagation as TDC is approached; and this effect is more pronounced for case 2 (hybrid combustion model). Comparisons between cases 1 and 2 of the turbulent kinetic energy profiles, the fuel vapor distributions and gas temperature profiles for each of these crankshaft angles indicate that the hybrid combustion model predicts faster burning rate in regions of high turbulent kinetic energy and temperature, and therefore less amounts of unburned fuel vapor are present in these regions. It would be expected that the turbulent mixing time (τ_t) would control the species conversion rates and energy release in these regions using the hybrid combustion model. As also seen in these figures, the regions marked by low turbulent kinetic energy (e.g., cylinder head and wall) are responsible for the poor mixing, and results in incomplete combustion as observed by high levels of unburned fuel vapor. These figures also show that the temperature profiles and unburned fuel vapor profiles near the cylinder head and wall are similar for case 1 (kinetics-controlled) and case 2 (hybrid combustion model). This is caused by the kinetics characteristic time (τ_q) controlling the species conversion rate

as the flame approaching the low temperature regions (cylinder head and wall), and similar predictions of the burning rate would be obtained using either the kinetics-controlled combustion model or the hybrid combustion model.

Some simplified observations can be made for the premixed-charge combustion engine flowfield. Premixed combustion results in rapid and high energy release (temperature rise) as seen in figure 2 (case 3) and more uniform burning. The burning rate (as observed by the isotherms) can be correlated with the spatial distribution of the turbulence in the engine. High turbulence intensity results in faster burning rate as observed by the hot flame kernel in the regions of high turbulent kinetic energy. As the premixed turbulent flame approaches the cylinder wall, piston face, and piston bowl, the decrease in turbulence intensity slows down the flame propagation resulting in slow and incomplete combustion in these regions (see figs. 2(b), (d), and (e), 3(b), (c), and (e), and 4(b), (d), and (e) for case 3).

At crankshaft angle about 15° ATDC, most of the liquid fuel has vaporized (cases 1 and 2) and most of the fuel (cases 1 to 3) has been depleted.

CONCLUSIONS

Kinetics-controlled combustion model and hybrid kinetics-mixing controlled combustion model have been used to make comparisons of mixing and burning rate. The comparisons have been made for a direct-injection stratified-charge combustion and a premixed-charge combustion gasoline fueled piston engines. The hybrid combustion model incorporates relaxation effects due to chemical kinetics and turbulent mixing times. The results obtained for the direct-injection stratified-charge combustion engine indicate that burning rate predicted by the hybrid combustion model is faster in regions of high turbulent kinetic energy, resulting in high temperature flame kernel and more depletion of the fuel. As the flame approaches the cylinder head and wall, the laminar kinetics time would eventually become controlling, thereby similar burning rate is obtained for the direct-injection stratified-charge engine using the kinetics-controlled or hybrid combustion model.

The hybrid combustion model with the same model constants has also been tested for a premixed-charge combustion engine and yielded reasonable results.

Future works will extend this hybrid combustion model to include more chemical species and the implementation of this combustion model into KIVA-II to study the combustion processes in High Speed Civil Transport and small gas turbine engines and to more accurately predict NO_x emission and unburned hydrocarbon.

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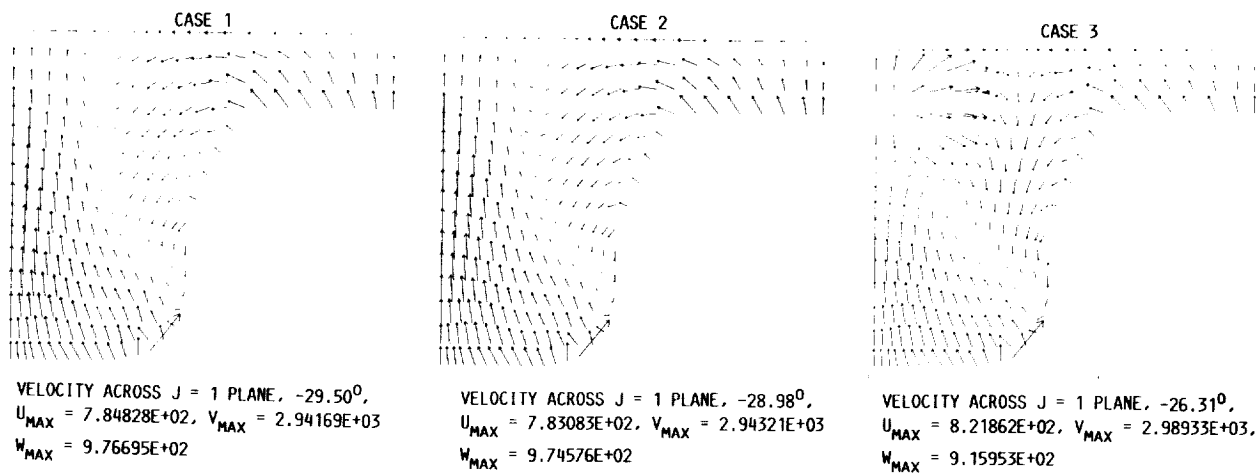
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TABLE I. - ENGINE PARAMETERS AND TEST CONDITIONS

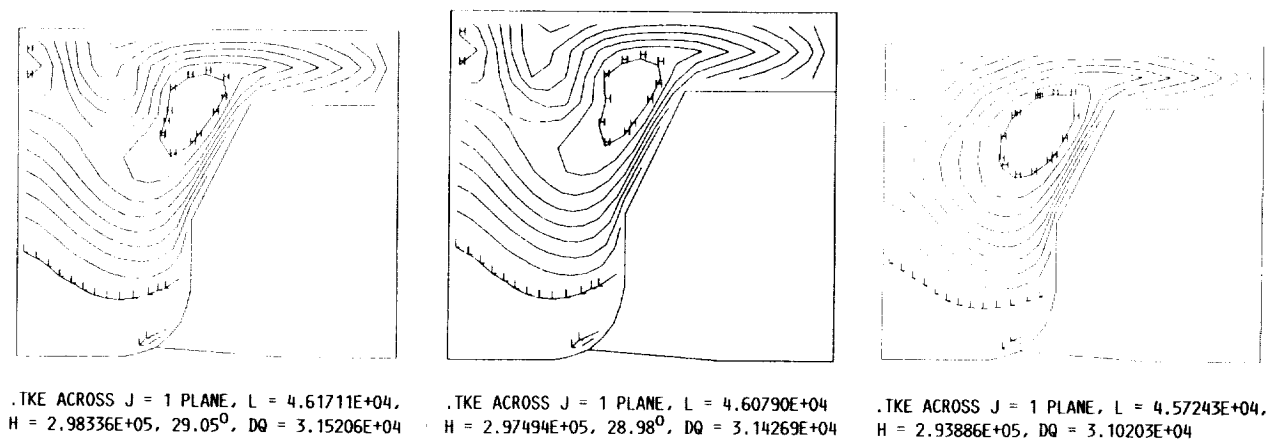
| | DISC engine | Premixed-charge combustion engine |
|--|-------------|--------------------------------------|
| Engine stroke, cm | 9.55 | 9.55 |
| Compression ratio | 6.54 | 6.54 |
| Volume of piston bowl, cm ³ | 58.8 | 58.8 |
| Squish clearance, cm | 0.1819 | 0.1819 |
| Connecting rod length, cm | 16.269 | 16.269 |
| rpm | 1600 | 1600 |
| Initial engine air temperature, K | 400 | 360 |
| Initial engine pressure, atm | 1 | 1 |
| Fuel | Isooctane | Isooctane |
| Starting crankangle of injection | 52° BTDC | ----- |
| Injection duration, deg | 12.672 | ----- |
| Injection angle, deg | 60 | ----- |
| Starting crankangle of ignition | 27° BTDC | ----- |
| Ignition duration, deg | 9.6 | ----- |

TABLE II. - MODEL CONSTANTS

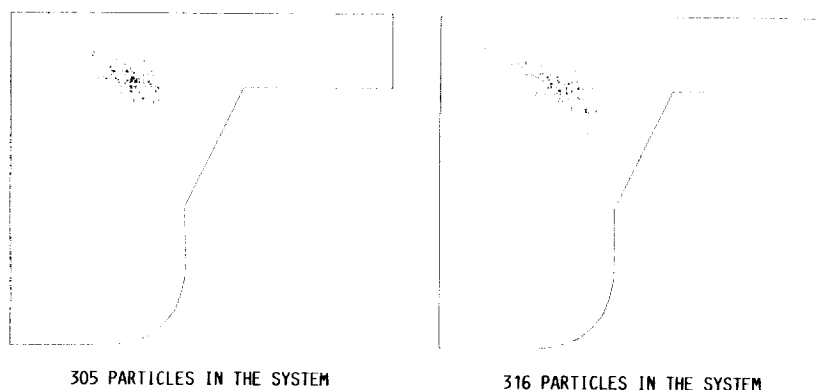
| |
|--|
| Turbulence: $C_1 = 1.44$; $C_2 = 1.92$; $C_3 = 1$ |
| Combustion model: $C_{m_1} = 2.75$; $C_{m_2} = 0.055$; $C_{m_3} = 0.092$; $B' = 4.59 \times 10^{-10}$ |
| $\xi = 1.0$; $\eta = -0.75$; $E_a/R = 15098$ K; $C = 0.08$ |



(a) GAS VELOCITY.



(b) TURBULENT KINETIC ENERGY.



(c) FUEL SPRAY.

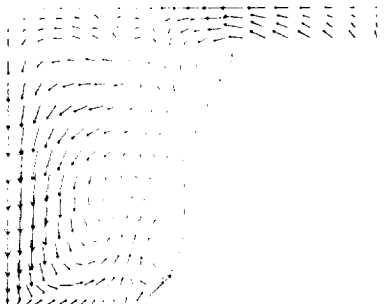
FIGURE 1. - RESULTS AT CRANKSHAFT ANGLE ABOUT 29° BTDC FOR CASE 1 (KINETICS-CONTROLLED COMBUSTION MODEL; DISC ENGINE), CASE 2 (HYBRID COMBUSTION MODEL; DISC ENGINE) AND CASE 3 (HYBRID COMBUSTION MODEL; PREMIXED CHARGE PISTON ENGINE).

CASE 1



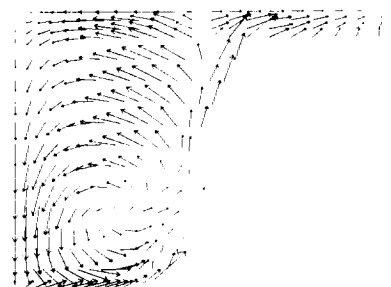
VELOCITY ACROSS J = 1 PLANE, -11.37° ,
 $U_{MAX} = 8.84606E+02$, $V_{MAX} = 3.38367E+03$,
 $W_{MAX} = 1.24565E+03$

CASE 2



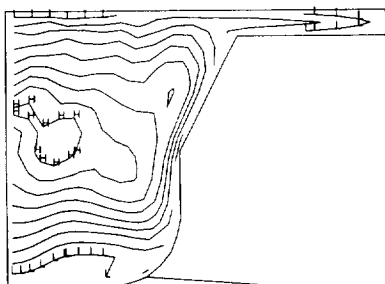
VELOCITY ACROSS J = 1 PLANE, -13.45° ,
 $U_{MAX} = 8.01494E+02$, $V_{MAX} = 3.23956E+03$,
 $W_{MAX} = 1.33204E+03$

CASE 3

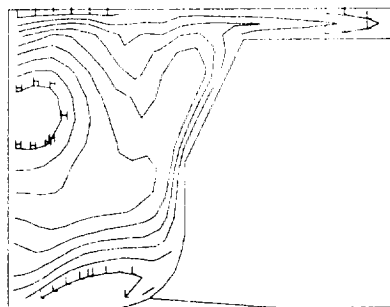


VELOCITY ACROSS J = 1 PLANE, -12.60° ,
 $U_{MAX} = 9.11390E+02$, $V_{MAX} = 2.72781E+03$,
 $W_{MAX} = 8.86937E+02$

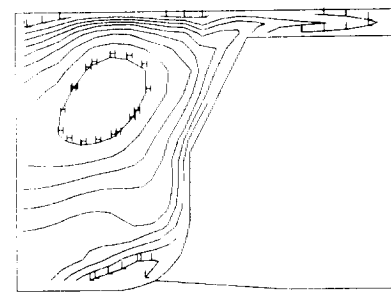
(a) GAS VELOCITY.



.TKE ACROSS J = 1 PLANE, $L = 4.80499E+04$,
 $H = 2.39197E+05$, -11.37° , $DQ = 2.38934E+04$

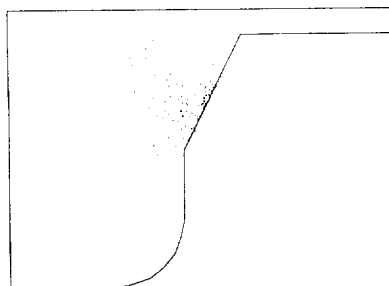


.TKE ACROSS J = 1 PLANE,
 $L = 5.38007E+04$, $H = 2.73481E+05$,
 -13.45° , $DQ = 2.74600E+04$

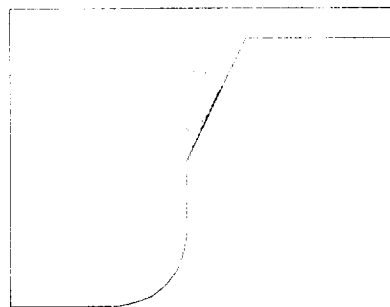


.TKE ACROSS J = 1 PLANE, $L = 6.56371E+04$,
 $H = 3.05680E+05$, -12.60° , $DQ = 3.00053E+04$

(b) TURBULENT KINETIC ENERGY.



122 PARTICLES IN THE SYSTEM

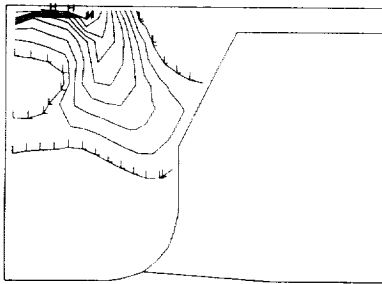


133 PARTICLES IN THE SYSTEM

(c) FUEL SPRAY.

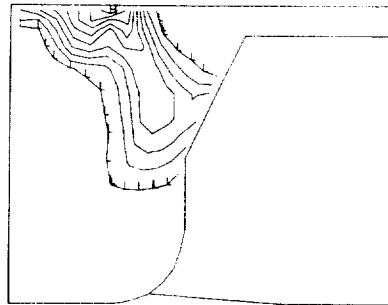
FIGURE 2. - RESULTS AT CRANKSHAFT ANGLE ABOUT 11° BTDC FOR CASES 1, 2, AND 3.

CASE 1



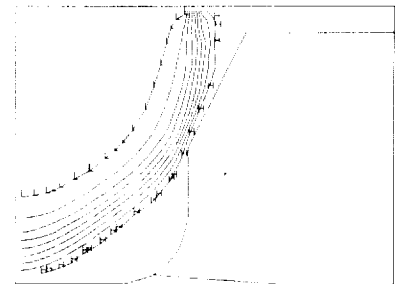
C_8H_{18} ACROSS J = 1 PLANE, L = 1.17529E-02,
H = 1.05776E-01, -11.37° , DQ = 1.17529E-02

CASE 2



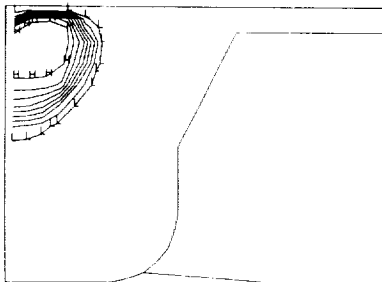
C_8H_{18} ACROSS J = 1 PLANE, L = 9.20729E-03,
H = 8.28655E-02, -13.45° , DQ = 9.20729E-03

CASE 3

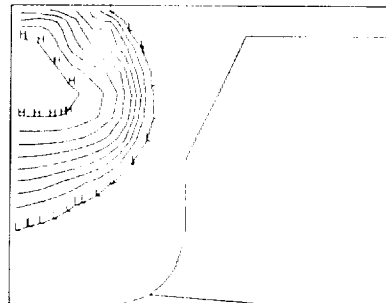


C_8H_{18} ACROSS J = 1 PLANE, L = 6.59493E+03,
H = 5.93543E+02, $150. -12.60^\circ$,
DQ = 6.59492E-03

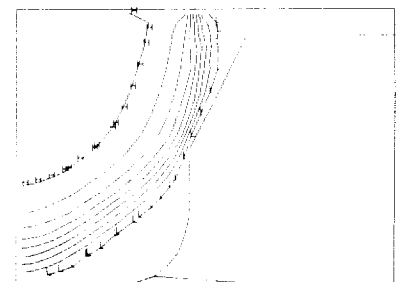
(d) FUEL VAPOR.



.TEMP ACROSS J = 1 PLANE, L = 6.57971E+02,
H = 2.96074E+03, -11.37° , DQ = 2.30277E+02



.TEMP ACROSS J = 1 PLANE, L = 7.127535+02,
H = 2.64682E+03, -13.45° , DQ = 1.93407E+02



.TEMP ACROSS J = 1 PLANE, L = 7.37012E+02,
H = 2.90261E+03, -12.60° , DQ = 2.16560E+02

(e) GAS TEMPERATURE.

FIGURE 2. - CONCLUDED.

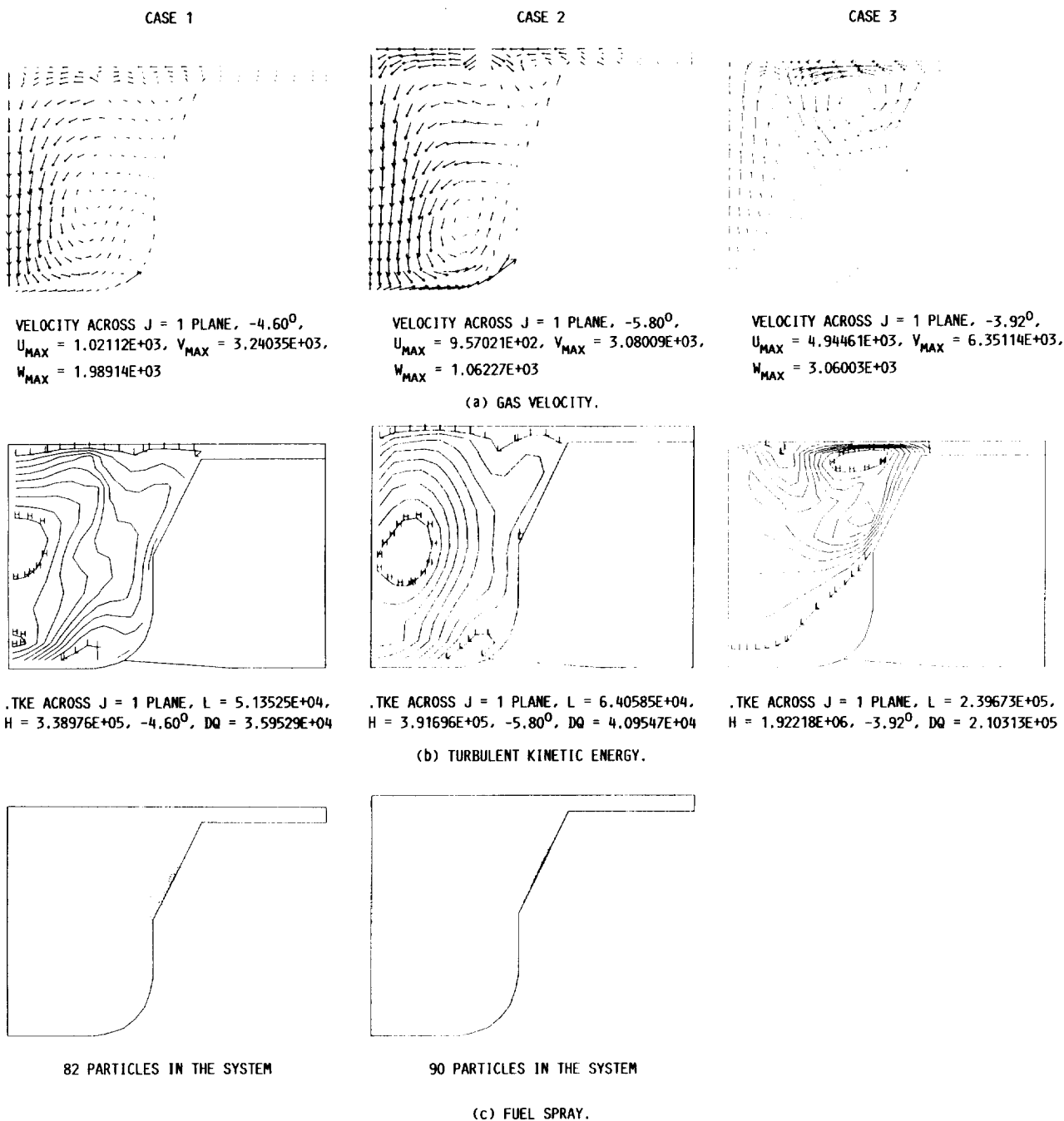
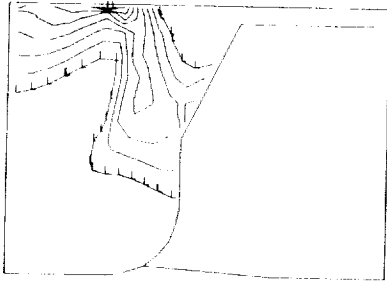


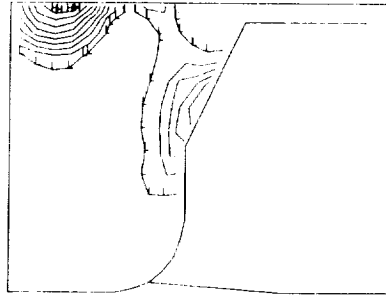
FIGURE 3. - RESULTS AT CRANKSHAFT ANGLE ABOUT 4° BTDC FOR CASES 1, 2 AND 3.

CASE 1



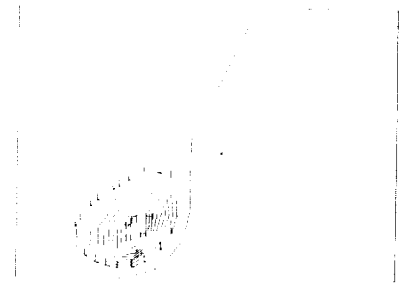
C_8H_{18} ACROSS J = 1 PLANE, L = 9.24640E-03,
H = 8.32176E-02, -4.60° , DQ = 9.24640E-03

CASE 2



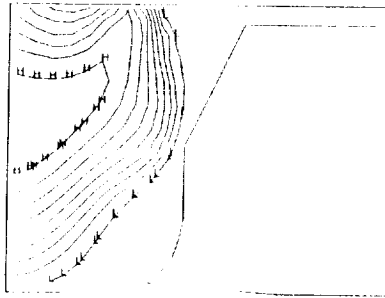
C_8H_{18} ACROSS J = 1 PLANE, L = 6.18474E-03,
H = 5.56626E-02, -5.80° , DQ = 6.18474E-03

CASE 3

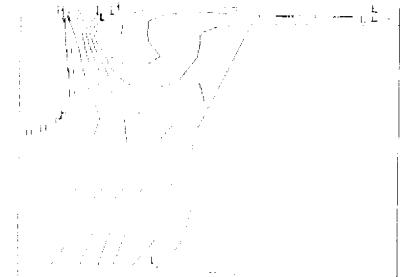


C_8H_{18} ACROSS J = 1 PLANE, L = 1.20906E-04,
H = 1.08816E-03, -3.92° , DQ = 1.20906E-04

(d) FUEL VAPOR.

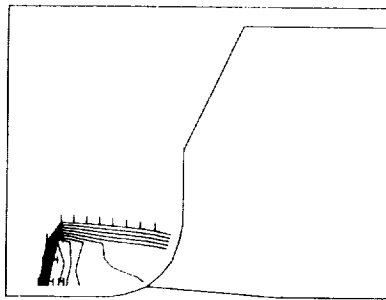


.TEMP ACROSS J = 1 PLANE, L = 7.91687E+02,
H = 2.76721E+02, -5.80° , DQ = 1.97553E+02



.TEMP ACROSS J = 1 PLANE, L = 2.63391E+03,
H = 3.32848E+03, -3.92° , DQ = 6.94568E+03

(e) GAS TEMPERATURE.



CO_2 ACROSS J = 1 PLANE, L = 9.68919E-03,
H = 8.72027E-02, -5.80° , DQ = 9.68919E-03



CO_2 ACROSS J = 1 PLANE, L = 7.70964E-03,
H = 6.93867E-02, -3.92° , DQ = 7.70964E-03

(f) CO_2 .

FIGURE 3. - CONCLUDED.

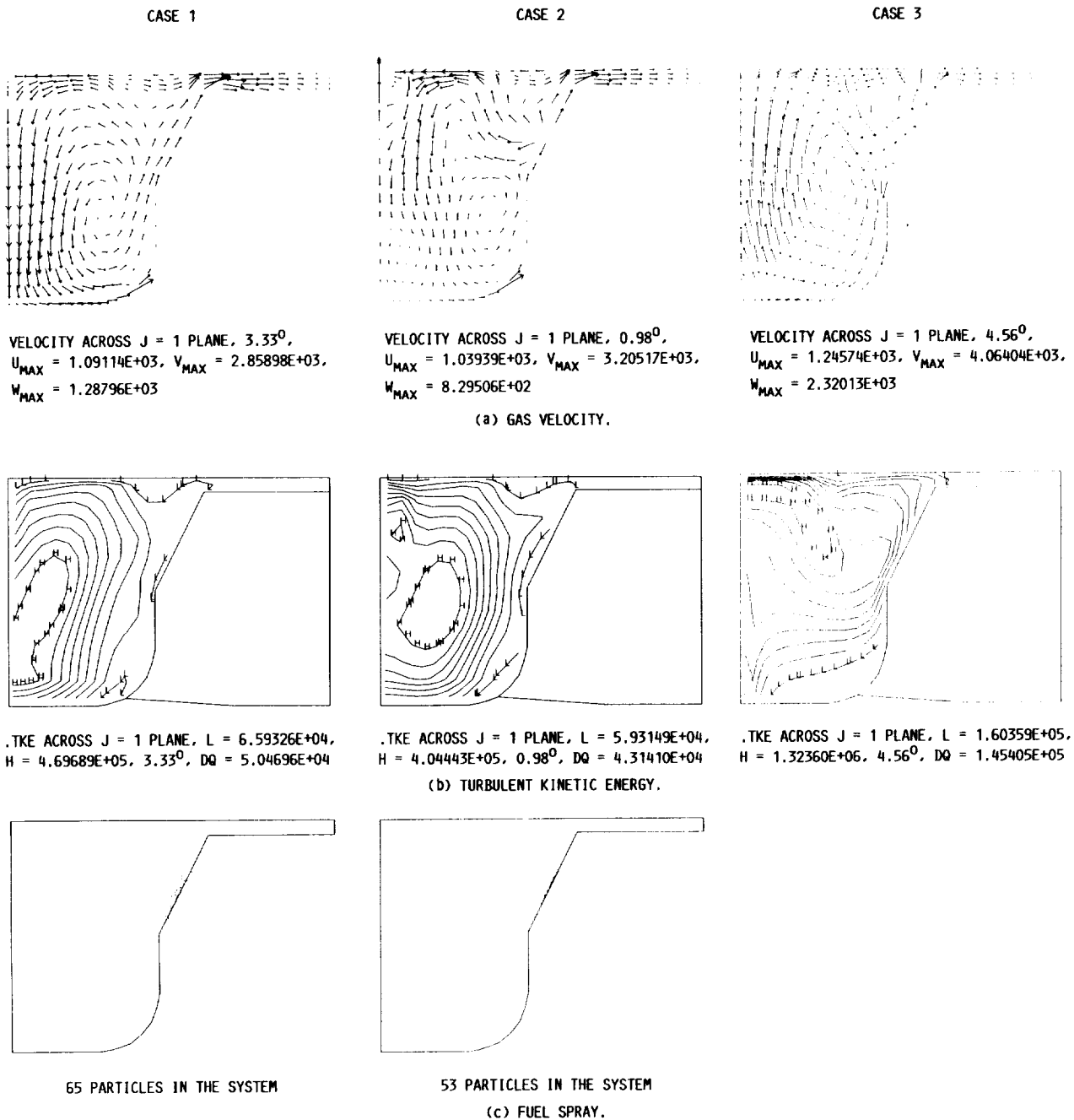
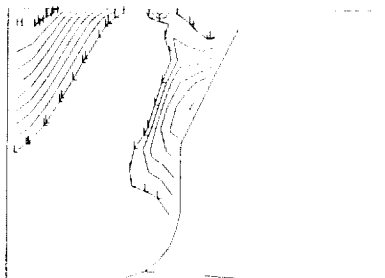


FIGURE 4. - RESULTS AT CRANKSHAFT ANGLE ABOUT 3° ATDC FOR CASES 1, 2 AND 3.

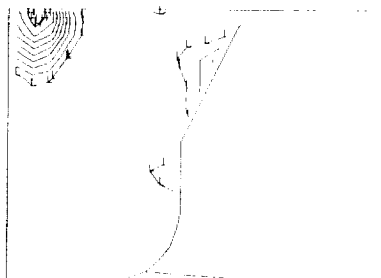
ORIGINAL PAGE IS
OF POOR QUALITY

CASE 1



$C_{8H_{18}}$ ACROSS J = 1 PLANE, L = 5.12489E-03,
H = 4.62591E-02, 3.33°, DQ = 5.14178E-03

CASE 2



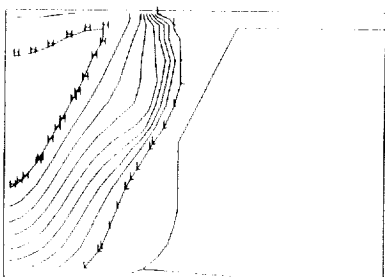
$C_{8H_{18}}$ ACROSS J = 1 PLANE, L = 5.23541E-03,
H = 4.71187E-02, 0.98°, DQ = 5.23541E-03

CASE 3

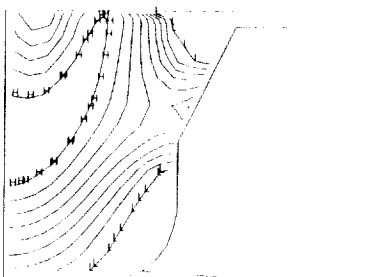


$C_{8H_{18}}$ ACROSS J = 1 PLANE, L = 1.76187E-07,
H = 1.58568E-06, 4.56°, DQ = 1.76187E-07

(d) FUEL VAPOR.



.TEMP ACROSS J = 1 PLANE, L = 7.95260E+02,
H = 3.00501E+03, 3.33°, DQ = 2.20976E+02

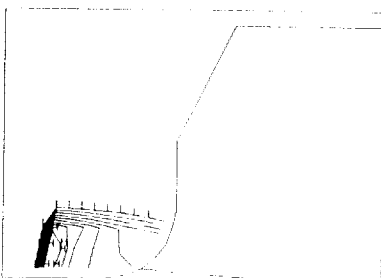


.TEMP ACROSS J = 1 PLANE, L = 8.33670E+02,
H = 2.80571E+03, 0.98°, DQ = 1.97204E+02

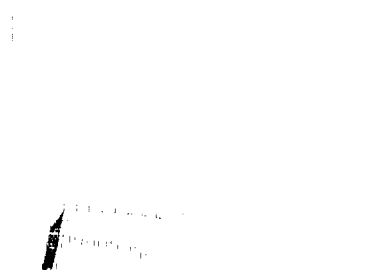


.TEMP ACROSS J = 1 PLANE, L = 2.49589E+03,
H = 3.20936E+03, 4.56°, DQ = 7.13467E+01

(e) GAS TEMPERATURE.



CO_2 ACROSS J = 1 PLANE, L = 1.04958E-02,
H = 9.44623E-02, 0.98°, DQ = 1.04958E-02



CO_2 ACROSS J = 1 PLANE, L = 7.43471E-03,
H = 6.69124E-02, 4.56°, DQ = 7.43471E-03

(f) CO_2 .

FIGURE 4. - CONCLUDED.

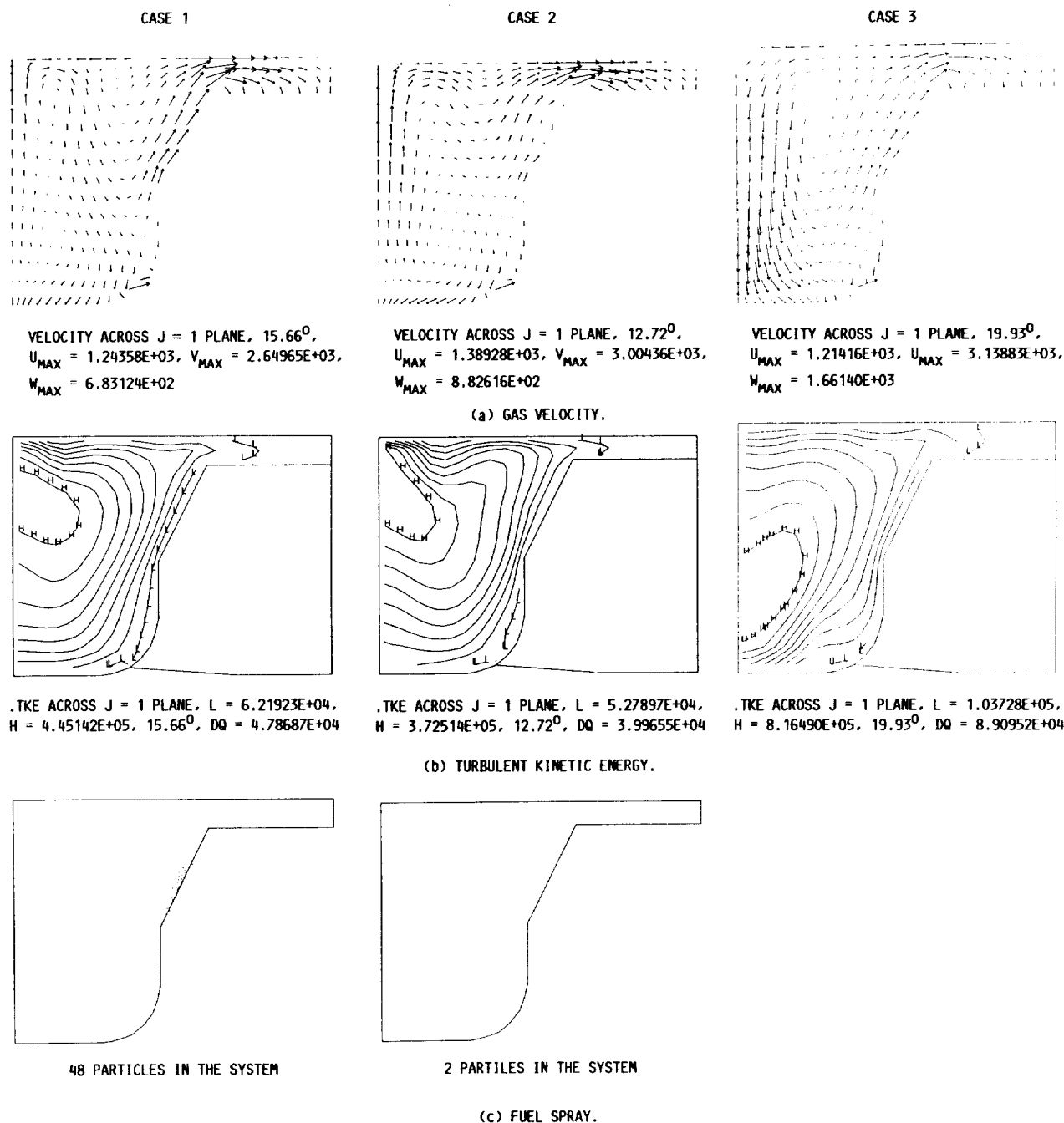
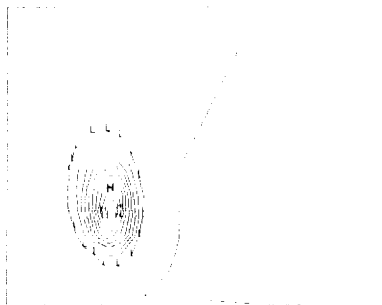


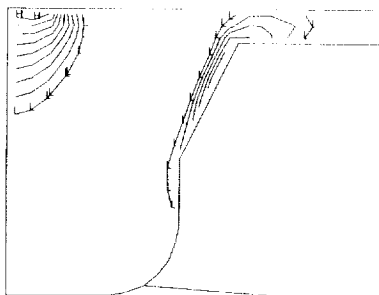
FIGURE 5. - RESULTS AT CRANKSHAFT ANGLE ABOUT 15° ATDC FOR CASES 1, 2 AND 3.

CASE 1



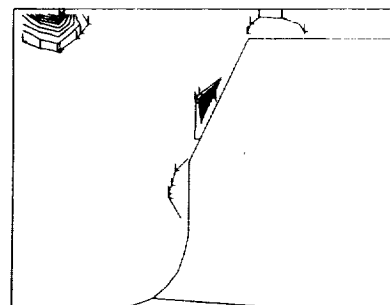
C_8H_{18} ACROSS J = 1 PLANE, L = 5.74846E-14,
H = 5.17576E-13, 19.93°, DQ = 5.75114E-14

CASE 2



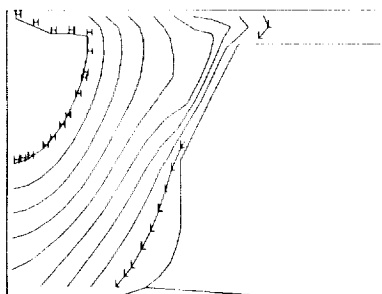
C_8H_{18} ACROSS J = 1 PLANE, L = 3.77290E-03,
H = 3.39584E-02, 15.66°, DQ = 3.77319E-03

CASE 3

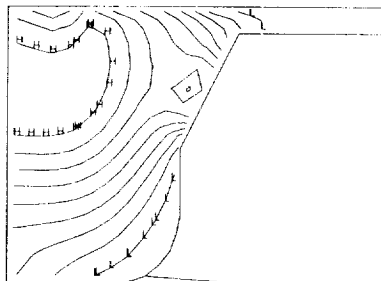


C_8H_{18} ACROSS J = 1 PLANE, L = 2.67012E-03,
H = 2.40307E-02, 12.72°, DQ = 2.67008E-03

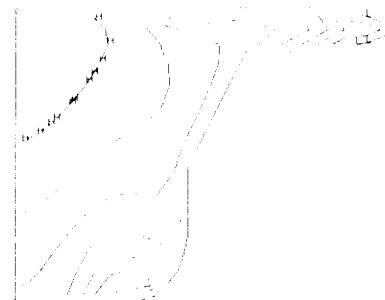
(d) GAS TEMPERATURE.



.TEMP ACROSS J = 1 PLANE, L = 7.61224E+02,
H = 2.82021E+03, 15.66°, DQ = 2.05899E+02

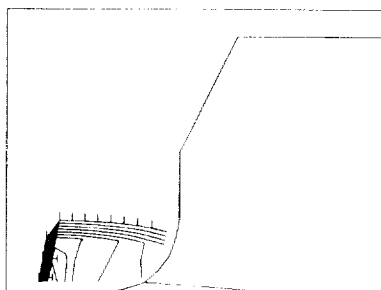


.TEMP ACROSS J = 1 PLANE, L = 7.88991E+02,
H = 2.67605E+03, 12.72°, DQ = 1.88706E+02



.TEMP ACROSS J = 1 PLANE, L = 2.15037E+03,
H = 2.89086E+03, 19.93°, DQ = 7.40485E+01

(e) GAS TEMPERATURE.



CO_2 ACROSS J = 1 PLANE, L = 1.11053E-02,
H = 9.99480E-02, 12.72°, DQ = 1.11053E-02



CO_2 ACROSS J = 1 PLANE, L = 1.03770E-02,
H = 9.33934E-02, 19.93°, DQ = 1.03770E-02

(f) CO_2 .

FIGURE 5. - CONCLUDED.

Report Documentation Page

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| | | | | 6. Performing Organization Code | |
| 7. Author(s) H. Lee Nguyen and Ming-Jyh Wey | | | | 8. Performing Organization Report No. E-5590 | |
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| 16. Abstract Two-dimensional calculations were made of spark-ignited premixed-charge combustion and direct-injection stratified-charge combustion in gasoline fueled piston engines. Results are obtained using kinetic-controlled combustion submodel governed by a four-step global chemical reaction or a hybrid laminar kinetics/mixing-controlled combustion submodel that accounts for laminar kinetics and turbulent mixing effects. In this work, the numerical solutions are obtained by using KIVA-II computer code. The KIVA-II code uses a kinetic-controlled combustion submodel governed by a four-step global chemical reaction; (i.e., it assumes that the mixing time is smaller than the chemistry). Our efforts involved the implementation of a hybrid laminar/mixing-controlled combustion submodel of Abraham et al. into KIVA-II. In this model, chemical species approach their thermodynamics equilibrium with a rate that is a combination of the turbulent-mixing time and the chemical-kinetics time. The combination is formed in such a way that the longer of the two times has more influence on the conversion rate and the energy release. An additional element of the model is that the laminar-flame kinetics strongly influence the early flame development following ignition. | | | | | |
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